

The ground state OH molecule in combined electric and magnetic fields: exact solution of the effective Hamiltonian

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The OH molecule is currently of great interest from the perspective of ultracold chemistry, quantum fluids, precision measurement and quantum computation. Crucial to these applications are the slowing, guiding, confinement and state control of OH, using electric and magnetic fields. In this Letter, we show that the corresponding eight-dimensional effective ground state Stark-Zeeman Hamiltonian is exactly solvable. Based on our solution, we analyze a waveguide for OH molecules. Our analytical result opens the way to insightful characterization of the magneto-electrostatic manipulation of ground state OH, and is also immediately applicable to other diatomic free radicals such as ClO, SF, NS, OD and SrF.

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The OH molecule in its ground $X^2\Pi_{3/2}$ state is presently widely employed in investigations of ultracold chemistry [1–4], precision measurements [5, 6], and quantum computation [7]. Particularly interesting is the recently implemented evaporative cooling of OH close to Bose-Einstein condensation [8]. With such experiments underway, the exploration of quantum degeneracy and molecular optics [9] with OH should shortly become reality.

A substantial reason behind the suitability of OH as a workhorse for the mentioned experiments is the fact that it is a polar paramagnetic molecule, i.e. it carries both electric and magnetic dipole moments. Electric and magnetic fields can therefore be used to slow, guide, confine and generally manipulate OH [10–14]. It follows that a quantitative as well as qualitative understanding of the corresponding Stark-Zeeman spectrum is of great relevance.

In this Letter we present the exact solution of the eight-dimensional Stark-Zeeman Hamiltonian of OH in its $X^2\Pi_{3/2}$ ground state [13]. This molecular Hamiltonian is an effective one, neglects hyperfine structure, and, to the best of our knowledge, has only been solved numerically [8, 12, 13]. Exact analytical solutions to a physical problem are of value because they describe how the system behaves in *any* regime, as opposed to numerical solutions, which usually describe a specific parameter range. During the preparation of this article, an analytical solution of the field-dependent part of the Hamiltonian was reported by Bohn *et al.* [15].

To demonstrate the usefulness of our solutions, we analyze a simple magneto-electrostatic waveguide for OH,

consisting of a current-carrying wire, a magnetic bias field, and an electric offset field [16]. We calculate analytically the energy minimum, trapping frequency, and anharmonicity of the waveguide as a function of the electric field. Using realistic parameters [8, 12, 13], we demonstrate the advantage of using an electric field in place of the standard magnetic offset field.

We expect that the solutions presented in this Letter can be used to construct an analytical yet realistic theory of nonadiabatic processes in traps, which so far has relied on the four-dimensional model of a fictitious $^2\Pi_{1/2}$ OH ground state [17]. Our work may also be of relevance to atmospheric [18], interstellar [19] and combustion physics [20], where OH plays an important role; and is immediately applicable to other molecules which have $^2\Pi_{3/2}$ Hund's case (a) states in their spectra, such as ClO, SF, NS, OD and SrF. Lastly, we hope that our discovery of an exactly solvable model will be of interest to physicists investigating the behavior of atoms and molecules in strong fields, and whose concerns include integrability and quantum chaos [21].

We begin with the Stark-Zeeman Hamiltonian for OH in the $X^2\Pi_{3/2}$ state, which has been derived earlier [13]

$$H = H_o - \vec{\mu}_e \cdot \vec{E} - \vec{\mu}_b \cdot \vec{B}, \quad (1)$$

where H_o is the field-free Hamiltonian, $\vec{\mu}_e$ and $\vec{\mu}_b$ are the electric and magnetic dipole moments of the molecule, respectively, and \vec{E} [\vec{B}] is the electric [magnetic] field imposed on the molecule. It has been shown that this model is valid when hyperfine structure is negligible, such as for electric fields stronger than 1kV/cm, and magnetic fields

above 100G [1]. For the present work, we will assume OH vapor temperatures higher than 2.7mK, in which case hyperfine structure can also be neglected [8, 13].

The matrix representation of the Hamiltonian in Eq. (1) can be obtained using the Hund's case (a) parity basis $|J, M, \bar{\Omega}, \epsilon\rangle$ suggested by Lara *et al.*, where $J = 3/2$ is the total angular momentum, M its projection in the

laboratory frame, $\bar{\Omega}$ its projection on the internuclear axis, and $\epsilon = \{e, f\}$ is the parity [17]. Following Ref.[17], both the electric and magnetic moments are assumed to lie along the axis of the molecule, and the magnetic field is chosen along the laboratory z axis, with which the electric field makes an angle θ . With these assumptions, the Hamiltonian matrix has been found to be [13]

$$H_M = \begin{pmatrix} -\frac{\hbar\Delta}{2} - \frac{6}{5}\mu_B B & 0 & 0 & 0 & \frac{3}{5}\mu_e E \cos \theta & -\frac{\sqrt{3}}{5}\mu_e E \sin \theta & 0 & 0 \\ 0 & -\frac{\hbar\Delta}{2} - \frac{2}{5}\mu_B B & 0 & 0 & -\frac{\sqrt{3}}{5}\mu_e E \sin \theta & \frac{1}{5}\mu_e E \cos \theta & -\frac{2}{5}\mu_e E \sin \theta & 0 \\ 0 & 0 & -\frac{\hbar\Delta}{2} + \frac{2}{5}\mu_B B & 0 & 0 & -\frac{2}{5}\mu_e E \sin \theta & -\frac{1}{5}\mu_e E \cos \theta & -\frac{\sqrt{3}}{5}\mu_e E \sin \theta \\ 0 & 0 & 0 & -\frac{\hbar\Delta}{2} + \frac{6}{5}\mu_B B & 0 & 0 & -\frac{\sqrt{3}}{5}\mu_e E \sin \theta & -\frac{3}{5}\mu_e E \cos \theta \\ \frac{3}{5}\mu_e E \cos \theta & -\frac{\sqrt{3}}{5}\mu_e E \sin \theta & 0 & 0 & \frac{\hbar\Delta}{2} - \frac{6}{5}\mu_B B & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{5}\mu_e E \sin \theta & \frac{1}{5}\mu_e E \cos \theta & -\frac{2}{5}\mu_e E \sin \theta & 0 & 0 & \frac{\hbar\Delta}{2} - \frac{2}{5}\mu_B B & 0 & 0 \\ 0 & -\frac{2}{5}\mu_e E \sin \theta & -\frac{1}{5}\mu_e E \cos \theta & -\frac{\sqrt{3}}{5}\mu_e E \sin \theta & 0 & 0 & \frac{\hbar\Delta}{2} + \frac{2}{5}\mu_B B & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{5}\mu_e E \sin \theta & -\frac{3}{5}\mu_e E \cos \theta & 0 & 0 & 0 & \frac{\hbar\Delta}{2} + \frac{6}{5}\mu_B B \end{pmatrix}, \quad (2)$$

where Δ is the lambda-doubling parameter, μ_B is the Bohr magneton, μ_e the molecular electric dipole moment, and E [B] are the magnitudes of the electric [magnetic] fields.

To the best of our knowledge, the matrix H_M of Eq.(2) has only been diagonalized numerically so far [8, 12, 13, 15]. We now show, remarkably, that this eight-dimensional Hamiltonian can be solved *analytically*. This can be seen by calculating the characteristic polynomial $P(\lambda)$ of H_M ,

$$P(\lambda) = |H_M - \lambda I| = \sum_{n=0}^8 p_n \lambda^n. \quad (3)$$

The coefficients of all the odd powers of λ vanish: $p_1 = p_3 = p_5 = p_7 = 0$. Thus, $P(\lambda)$, which is an octic in λ , can be written as a quartic in λ^2 ,

$$P(\lambda) = p_0 + p_2 \lambda^2 + p_4 (\lambda^2)^2 + p_6 (\lambda^2)^3 + p_8 (\lambda^2)^4, \quad (4)$$

and therefore its roots can be found analytically [22]. Expressions for the coefficients p_n and eigenvalues $E_{M,\epsilon}$ of Eq. (3) are most readily obtained using *Mathematica* and are provided in the Supplementary Material. The eigenvalue of interest in this article, $E_{3/2,f}$, can be written as

$$E_{3/2,f} = \sqrt{-\frac{p_6}{4} + \frac{\sqrt{g_1}}{2} + \frac{\sqrt{g_2 + g_3}}{2}}, \quad (5)$$

where

$$\begin{aligned} g_1 &= -\frac{2p_4}{3} + \frac{p_6^2}{4} + \frac{2^{1/3}h_2}{3h_3} + \frac{h_3}{2^{1/3}}, \\ g_2 &= -\frac{4p_4}{3} + \frac{p_6^2}{2} - \frac{2^{1/3}h_2}{3h_3} - \frac{h_3}{2^{1/3}}, \\ g_3 &= \frac{-8p_2 + 4p_4p_6 - p_6^3}{4\sqrt{g_1}}, \\ h_1 &= 27p_2^2 - 72p_0p_4 + 2p_4^3 - 9p_2p_4p_6 + 27p_0p_6^2, \\ h_2 &= 12p_0 + p_4^2 - 3p_2p_6, \\ h_3 &= \left(h_1 + \sqrt{h_1^2 - 4h_2^3}\right)^{1/3}. \end{aligned} \quad (6)$$

We have verified that the analytical eigenvalues, displayed in Fig. 1, reproduce exactly the purely numerically obtained OH spectra, as in Ref.[13], for example. We note that although it is conventional and useful to label the eigenvalues using the angular momentum projection M and the parity ϵ , neither is a good quantum number [13].

As expected from Eq. (4) and shown in Fig. 1, the spectrum is vertically symmetric about zero energy, i.e. if λ is an eigenvalue, so is $-\lambda$. The observation of this symmetry in the numerically generated spectra [13] was the crucial step in arriving at the analytical solution of the problem. This kind of symmetry seems to have been noticed in only a handful of physical systems [23]. Perhaps the best known example is that of a free Dirac particle, where the 'reflection' symmetry of the spectrum follows from

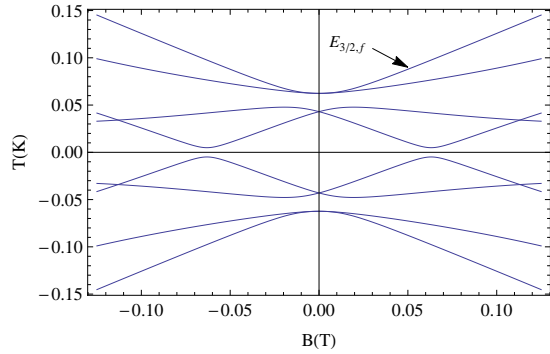


FIG. 1: Plot of the analytical eigenvalues of OH with the parameters $\Delta = 2\pi \times 1.667\text{GHz}$, $\mu_e = 1.66\text{D}$, $E = 2\text{kV/cm}$, and $\theta = \pi/2$. The horizontal axis denotes the magnetic field in Tesla and the vertical axis corresponds to energy in units of temperature. For clarity, only the state $E_{3/2,f}$ currently used for trapping OH [12, 13] has been labeled.

the anticommutation of the charge conjugation operator with the corresponding Hamiltonian [24]. In the present case, the physical origin of this spectral symmetry is not clear, partly due to the effective nature of the Hamiltonian, and is an open and interesting question posed by our work.

We now demonstrate how our solutions can be used to analytically characterize magneto-electrostatic manipulation of OH molecules. The dramatic influence of electric fields on magnetic OH traps has recently been demonstrated experimentally, in terms of increasing steady-state trap population [12], as well as implementing evaporative cooling [8]. These experimental configurations are quite complicated and will be considered in the context of our analytical solutions in future work. In the present article, we examine instead a simpler geometry. Particularly, we are interested in the effect of an electric field on a magnetic waveguide for OH. Such an electric field could be useful for polarizing the OH electric dipole, or for manipulating cold collisions [1, 2].

We first briefly review the standard magnetic quadrupole waveguide configuration, which can be used to guide any paramagnetic molecule, including OH [16]. As shown in Fig. 2, the guide consists of a wire carrying a current I in the z direction (i.e. out of the page), and a homogeneous magnetic bias field B_b in the x direction. We have chosen this configuration since it is analytically simple to model. The resulting magnetic field away from the origin is given by

$$\vec{B}_t = \left[B_b - \frac{\mu_0 I y}{2\pi(x^2 + y^2)} \right] \hat{x} + \frac{\mu_0 I x}{2\pi(x^2 + y^2)} \hat{y}, \quad (7)$$

and has a zero at $x_o = 0$ and $y_o = \mu_0 I / (2\pi B_b)$. Para-

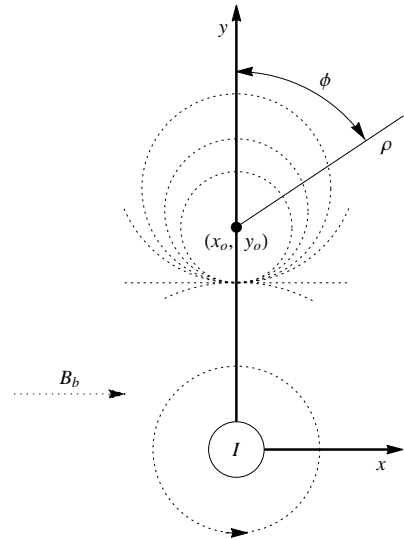


FIG. 2: Schematic of the OH magneto-electrostatic guide considered in this work. Included in the diagram are a wire carrying current I along the z axis out of the page, and a magnetic bias field B_b along the x axis. Their superposition results in a quadrupole guide at the location marked (x_o, y_o) . Any point in the guide can be labeled using the coordinates ρ and ϕ , as shown. In the standard configuration, a magnetic offset field B_o along the z axis is also used. We consider in this work instead an electric field E , applied in the same direction.

magnetic atoms and molecules can be guided along this line, parallel to the z axis. Shifting the origin to the point (x_o, y_o) , the magnitude of the magnetic field can be written as [16]

$$|\vec{B}_t| = \frac{B_b \rho}{\sqrt{\rho^2 + y_o^2 + 2\rho y_o \cos \phi}}, \quad (8)$$

where the radial distance ρ and the angle ϕ are measured as shown in Fig. 2. For $\rho \ll y_o$, Eq. (8) is radially symmetric about (x_o, y_o) . Thus, we may simply write $|\vec{B}_t| \simeq b\rho$, where $b = B_b/y_o$ is the magnetic field gradient at the guide center.

One of the problems with this configuration is that due to the zero field at the trap center ($\rho = 0$) Majorana losses can occur [16]. In order to prevent such losses, usually a magnetic offset field B_o along the z axis is applied, resulting in a total field magnitude $B(\rho) = (|\vec{B}_t|^2 + B_o^2)^{1/2}$. Assuming, as in current experiments, that the $E_{3/2,f}$ internal state is used for guiding OH [13], the potential energy of the molecule near the guide center can be written as a Taylor expansion of the exact eigenvalue

$$E_{3/2,f}(\rho) = E_{3/2,f}^{(0)}(0) + E_{3/2,f}^{(1)}(0)\rho + E_{3/2,f}^{(2)}(0)\rho^2 + \dots \quad (9)$$

In Eq. (9), $E_{3/2,f}^{(n)}(0) = (n!)^{-1} \partial^n E_{3/2,f}(\rho) / \partial \rho^n|_{\rho=0}$. Further, the energy depends only on ρ since the system is cylindrically symmetric about, and translationally invariant along, the z axis. Lastly, except at the guide center, the net magnetic field does not point along the z axis, thus apparently contravening the convention of Eq. (2). However, in that case a new z axis can readily be chosen in the direction of the local magnetic field, and the procedure yields the same results as presented below.

The required eigenvalue for this case can be found directly by setting $E = 0$ in Eq. (2), which then takes a diagonal form. Using the resulting solution $E_{3/2,f}(\rho) = \hbar\Delta/2 + 6\mu_B B(\rho)/5$, we find that $E_{3/2,f}^{(0)}(0) = \hbar\Delta/2 + 6\mu_B B_o/5$, implying that the nonzero magnetic field at the guide center interacts with the OH molecule, thus lowering Majorana losses. Further, we find $E_{3/2,f}^{(1)}(0) = 0$ and $E_{3/2,f}^{(2)}(0) = 3\mu_B b^2/5B_o$, making the trap harmonic to lowest order in ρ . Lastly, $E_{3/2,f}^{(3)}(0) = 0$ and $E_{3/2,f}^{(4)}(0) = -3\mu_B b^4/20B_o^3$. Thus, the lowest order, i.e. quartic, anharmonicity cannot be fully removed, although it can be reduced in magnitude by choosing a small b and a large B_o .

We now consider the effect of replacing the magnetic offset field B_o by a homogeneous electric field E , also applied in the z direction [8, 13], which conserves the cylindrical symmetry of the system. Using a realistic simulation, we have confirmed that for the parameters presented in this Letter the electric field near the guide center is only negligibly perturbed by the presence of the wire. The quantities relevant to guiding can be found from Eq. (5) with $E \neq 0$, $\theta = \pi/2$, and Eq. (9); such a treatment is equivalent to choosing a molecular z axis along the direction of the local magnetic field.

We find that the energy at the guide center is given exactly by

$$E_{3/2,f}^{(0)}(0) = \left[\left(\frac{\hbar\Delta}{2} \right)^2 + \left(\frac{3\mu_e E}{5} \right)^2 \right]^{1/2}. \quad (10)$$

The non-zero electric field at the trap minimum thus provides the molecule with a quantization axis and may be expected to mitigate Majorana losses [15]. We note that the first derivative in Eq. (9) vanishes, i.e. $E_{3/2,f}^{(1)}(0) = 0$, making the trap harmonic to lowest order in ρ . The guide frequency $\nu_\rho = [2E_{3/2,f}^{(2)}(0)/m]^{1/2}/2\pi$, where m is the mass of the OH molecule, is found to be

$$\nu_\rho = \frac{b}{2\pi} \left[\frac{6\mu_B^2 [(5\hbar\Delta)^2 + 24(\mu_e E)^2]}{10m(\mu_e E)^2 [(5\hbar\Delta)^2 + (6\mu_e E)^2]^{1/2}} \right]^{1/2}, \quad (11)$$

and is plotted in Fig. 3(a) for realistic parameters.

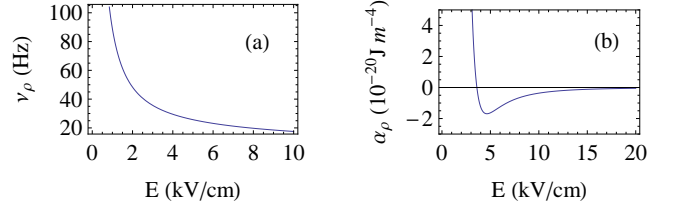


FIG. 3: (a) The frequency and (b) anharmonicity of the guide in Fig.2 as a function of the electric field. Parameters used are $I = 1500A$, $B_b = 0.03T$, $m = 17amu$, $\Delta = 2\pi \times 1.66GHz$, and $\mu_e = 1.667D$ [13], implying $y_o = 10mm$ and $b = 3T/m$.

Next, we examine the trap anharmonicity. The cubic anharmonicity is identically zero, while the quartic contribution α_ρ can be found analytically to be $\alpha_\rho = F/G$, where $F = 3(5\hbar\Delta)^6 + 57(5\hbar\Delta)^4(2\mu_e E)^2 + 216(5\hbar\Delta)^2(2\mu_e E)^4 - 648(2\mu_e E)^6$, and $G = \frac{5}{2}(2\mu_e E)^6[9(2\mu_e E)^2 + (5\hbar\Delta)^2]^{3/2}$. The denominator G is always positive, but the presence of the last negative term in the numerator F immediately suggests that the anisotropy can be removed by choosing the electric field magnitude appropriately. Indeed, Fig. 3(b) shows that the OH guide anharmonicity vanishes at about $E = 3.5kV/cm$. Choosing this value of the field might be useful as the effect of the anharmonic term can be quite large; at $E = 500V/cm$, and $\rho = 2mm$ it equals 20% that of the harmonic potential energy. Finally, for completeness, the depth of the guide as a function of the electric field has been provided in the Supplementary Material.

Before concluding, we note two subtle points. First, at the center of the guide, $B = 0$, leading to θ being undefined in Eq. (2). However, this is not a problem, as Eq. (10) can be shown to hold for any θ , and the expressions for the frequency and anharmonicity presented above can be recovered in the limit of arbitrarily small (but nonzero) B close to the guide center. Second, we note that both the guide frequency and anharmonicity diverge as $E \rightarrow 0$. This is due to the avoided crossing turning into a crossing, and introducing a discontinuity in the derivatives of the Taylor expansion of Eq. (9). At $E = 0$, the transverse character of the guide changes fundamentally, from harmonic to linear.

In conclusion, we have solved exactly the effective Hamiltonian of the $X^2\Pi_{3/2}$ state Hund's case (a) molecule in combined electric and magnetic fields, neglecting hyperfine structure. In the context of a realizable waveguide, we have shown that our results allow insightful analytic characterization of the magneto-electrostatic manipulation of OH molecules. Our analysis can readily be extended to other field configurations [11, 12] and other molecules such as ClO, SF, NS, OD and SrF.

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Supplementary Material for “The ground state OH molecule in combined electric and magnetic fields: exact solution of the effective Hamiltonian”

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Below we provide additional details of the calculations presented in the main article. The analytical as well as numerical calculations were carried out using *Mathematica*; a notebook containing these results is available upon request to mxbsps@rit.edu.

A. Coefficients of the characteristic polynomial

The coefficients p_n in Eq.(3) of the main article are found to be

$$p_1 = p_3 = p_5 = p_7 = 0, \quad (1)$$

and

$$p_0 = \frac{1}{10^8} \left\{ 81\tilde{B}^8 + 324\tilde{B}^4\tilde{E}^4 + 81\tilde{E}^8 - 180\tilde{B}^6\tilde{\Delta}^2 + 756\tilde{B}^4\tilde{E}^2\tilde{\Delta}^2 - 756\tilde{B}^2\tilde{E}^4\tilde{\Delta}^2 \right. \\ \left. + 180\tilde{E}^6\tilde{\Delta}^2 + 118\tilde{B}^4\tilde{\Delta}^4 - 264\tilde{B}^2\tilde{E}^2\tilde{\Delta}^4 + 118\tilde{E}^4\tilde{\Delta}^4 - 20\tilde{B}^2\tilde{\Delta}^6 + 20\tilde{E}^2\tilde{\Delta}^6 + \tilde{\Delta}^8 \right. \\ \left. - 4\tilde{B}^2\tilde{E}^2 \left(81\tilde{B}^4 + 81\tilde{E}^4 + 54\tilde{B}^2\tilde{\Delta}^2 - 54\tilde{E}^2\tilde{\Delta}^2 - 7\tilde{\Delta}^4 \right) \cos 2\theta + 162\tilde{B}^4\tilde{E}^4 \cos 4\theta \right\}, \quad (2)$$

$$p_2 = \frac{1}{50000} \left\{ -9\tilde{B}^6 - 9\tilde{E}^6 - \frac{1}{5}\tilde{\Delta}^6 - \frac{59}{5}\tilde{E}^4\tilde{\Delta}^2 - 3\tilde{E}^2\tilde{\Delta}^4 - 9\tilde{B}^4\tilde{E}^2 - \frac{23}{5}\tilde{B}^4\tilde{\Delta}^2 - 9\tilde{B}^2\tilde{E}^4 \right. \\ \left. + \tilde{B}^2\tilde{\Delta}^4 + \frac{48}{5}\tilde{B}^2\tilde{E}^2\tilde{\Delta}^2 + 2\tilde{B}^2\tilde{E}^2 \left(9\tilde{B}^2 + 9\tilde{E}^2 + \frac{17}{5}\tilde{\Delta}^2 \right) \cos 2\theta \right\}, \quad (3)$$

$$p_4 = \frac{1}{5000} \left\{ 59\tilde{B}^4 + 36\tilde{B}^2\tilde{E}^2 + 10\tilde{B}^2\tilde{\Delta}^2 - 82\tilde{B}^2\tilde{E}^2 \cos 2\theta + 59\tilde{E}^4 + 30\tilde{E}^2\tilde{\Delta}^2 + 3\tilde{\Delta}^4 \right\}, \quad (4)$$

$$p_6 = -\frac{1}{5} \left\{ \tilde{B}^2 + \tilde{E}^2 + \frac{1}{5}\tilde{\Delta}^2 \right\}, \quad (5)$$

$$p_8 = 1. \quad (6)$$

where $\tilde{B} = 4\mu_B B$, $\tilde{E} = 2\mu_e E$, and $\tilde{\Delta} = 5\hbar\Delta$. (Continued on the next page).

B. Eigenvalues

The roots of the characteristic polynomial of Eq. (4) in the main article are found most directly in analytic form using *Mathematica*, and are given below:

$$E_{3/2,f} = \sqrt{-\frac{p_6}{4} + \frac{\sqrt{g_1}}{2} + \frac{\sqrt{g_2 + g_3}}{2}}, \quad (7)$$

$$E_{3/2,e} = \sqrt{-\frac{p_6}{4} + \frac{\sqrt{g_1}}{2} - \frac{\sqrt{g_2 + g_3}}{2}}, \quad (8)$$

$$E_{1/2,f} = \sqrt{-\frac{p_6}{4} - \frac{\sqrt{g_1}}{2} + \frac{\sqrt{g_2 - g_3}}{2}}, \quad (9)$$

$$E_{1/2,e} = \sqrt{-\frac{p_6}{4} - \frac{\sqrt{g_1}}{2} - \frac{\sqrt{g_2 - g_3}}{2}}, \quad (10)$$

$$E_{-1/2,f} = -E_{1/2,e}, \quad (11)$$

$$E_{-1/2,e} = -E_{1/2,f}, \quad (12)$$

$$E_{-3/2,f} = -E_{3/2,e}, \quad (13)$$

$$E_{-3/2,e} = -E_{3/2,f}, \quad (14)$$

$$\begin{aligned} g_1 &= -\frac{2p_4}{3} + \frac{p_6^2}{4} + \frac{2^{1/3}h_2}{3h_3} + \frac{h_3}{2^{1/3}3}, \\ g_2 &= -\frac{4p_4}{3} + \frac{p_6^2}{2} - \frac{2^{1/3}h_2}{3h_3} - \frac{h_3}{2^{1/3}3}, \\ g_3 &= \frac{-8p_2 + 4p_4p_6 - p_6^3}{4\sqrt{g_1}}, \\ h_1 &= 27p_2^2 - 72p_0p_4 + 2p_4^3 - 9p_2p_4p_6 + 27p_0p_6^2, \\ h_2 &= 12p_0 + p_4^2 - 3p_2p_6, \\ h_3 &= \left(h_1 + \sqrt{h_1^2 - 4h_2^3} \right)^{1/3}. \end{aligned} \quad (15)$$

The Taylor series expansions provided in the article were obtained using *Mathematica* and the validity of the Taylor series up to the required number of terms was established by comparison with the full numerical solution for specific parameters.

C. Reflection symmetry in the spectrum

In the spectrum of the OH molecule, if λ is an eigenvalue, so is $-\lambda$, as shown in Fig.1 in the main article. In many systems that exhibit such a feature, the symmetry of the spectrum follows from the existence of an operator C that anticommutes with the system Hamiltonian H_S , i.e.

$$CH_S + H_SC = 0, \quad (16)$$

If we consider an eigenvector ψ_+ with an eigenvalue E , we can write $H_S\psi_+ = E\psi_+$. Multiplying from the left by C and rearranging, we find $CH_S\psi_+ = EC\psi_+$. Finally, using the anticommutation, we arrive at

$$H_S(C\psi_+) = -E(C\psi_+). \quad (17)$$

This implies that $C\psi_+$ is an eigenfunction of H_S with an eigenvalue $-E$. The existence of the operator C thus leads to the $\pm E$ pairing of eigenvalues in the energy spectrum. Assuming C is invertible we can write Eq. (16) as

$$CH_SC^{-1} = -H_S, \quad (18)$$

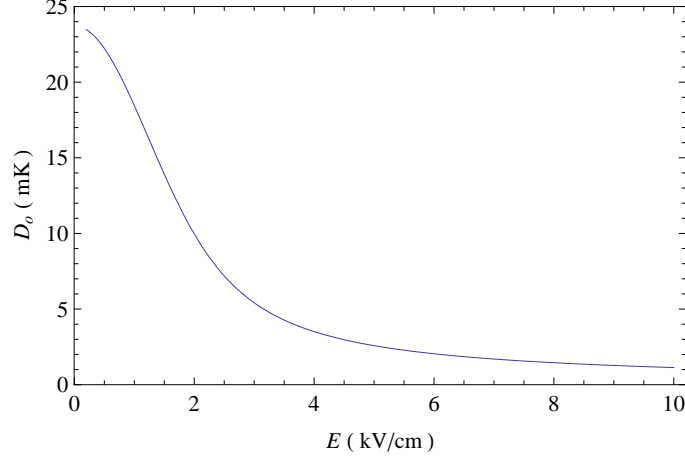


FIG. 1: The transverse depth of the guide as a function of the electric field. Parameters used are $I = 1500A$, $B_b = 0.03T$, $m = 17\text{amu}$, $\Delta = 2\pi \times 1.66\text{GHz}$, $\mu_e = 1.667D$, implying $y_o = 10\text{mm}$ and $b = 3T/m$, and $Y = 100y_o$.

meaning that the operation C simply changes the sign of the Hamiltonian. A matrix representation for C can readily be found for the diagonal form of our molecular Hamiltonian H_M ,

$$C = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}. \quad (19)$$

A physical interpretation of C remains to be found.

D. Guide depth as a function of the electric field

The guide depth can be found from Eqs. (5) and (7) of the main article which can be used to find the Stark-Zeeman energy $E_{3/2,f}(x, y)$. The guide depth can then be defined as

$$D_o = E_{3/2,f}(0, Y) - E_{3/2,f}(x_o, y_o), \quad (20)$$

where $Y \gg y_o$ is a coordinate far away from the guide center. A plot of D_o is shown in Fig.1 of this Supplement. As can be seen from the figure, for the field value at which anisotropy is exactly canceled [$E \simeq 3.5\text{kV/cm}$, see Fig.2(b) in the main article], the trap depth is larger than 2.7mK , which is the minimum OH temperature required for Eq.(2) of the main article to be valid.